THE INFLUENCE OF ATOMIC DEFECTS ON THE MECHANICAL PROPERTIES AND BREAKING BEHAVIORS OF GOLD NANOWIRES

Fenying Wang* [a)], Yanfeng Dai*, Qianjin Li** & Jianwei Zhao**
*Education Center for Basic Chemistry Experiments, Chemistry Department, School of Science, Nanchang University, Nanchang , 330031, China
**State Key Laboratory of Analytical Chemistry for Life Science, School of Chemistry and Chemical Engineering,Nanjing University, Nanjing, 210008, China

Summary The mechanical properties and breaking behaviors of the [100] oriented single-crystal gold nanowires containing a set of defect ratios have been studied using molecular dynamics simulations at different temperatures. The breaking behaviors of nanowires subjected to uniaxial tension have been found to present a statistic feature. It indicates analyzing of enormous samples might be the only way to investigate the material failure in the nanoscale devices. While the size of the device component reaches several nanometers, the existence of atomic defects has been expected to be more profound in dominating the device failure. When the defects are constructed, the improving mechanical strengths of nanowires decrease with the temperature increasing. Comparing to the perfect nanowire, the existence of the atomic defects extends the elastic deformation showing a larger yield strain. When the defect ratio is 5% at 100 K, the nanowire breaking behavior is sensitive to the atomic defects. However, the ratio is 1% when temperatures are 300 and 500 K.

INTRODUCTION

In recent years, mechanical properties of the metallic nanowires are of considerable interests due to its potential applications in electronic and electromechanical devices. For the mechanical strength and breaking behavior/failures of nanowires subjected to uniaxial stretching, it could be affected by many factors, such as stretching rates, size, defects, crystalline orientation and temperature. With experimental methods, mechanical measurements of individual nanowires are challenging, principally owing to some difficulties in performing standard tensile or bending tests on the nanoscale systems. It is also a problem to study the deformation mechanisms, mechanical strength and breaking behavior of the nanowire containing different defects ratios at different measuring conditions. Theoretical simulations, especially for molecular dynamics (MD) simulations, have been demonstrated to be powerful to evaluate the properties of nanowires subjected to mechanical stretching. With MD simulations, a profound understanding about mechanical properties of the nanowire will be helpful for designing, manufacturing, and manipulating the metallic nanowire before the nanowire is successfully incorporated into the active component of nanoelectromechanical system (NEMS) devices.

METHODOLOGY

As is shown in Fig. 1, the gold nanowire subjected to uniaxial tension was generated as a regular lattice of face centered cubic (FCC) along the [100] crystallographic orientation. The size was 10a × 10a × 30a (a stands for lattice constant, 0.408 nm for gold). Ten different temperatures were set from 5 to 750 K. At each temperature, 300 initial equilibrium states with different atomic configuration were adopted for the nanowire using different and enough relax time, which were appropriate to ensure the reliability of MD simulations. In all, 8,700 (29×300) samples were used to give the insight into the defect effects as well as the temperature effect on the mechanical properties and breaking behavior of the single-crystal gold nanowire.Using statistical analysis, the most probable breaking position (MPBP) is obtained from the fitting peak of breaking position distribution of the perfect single-crystal gold nanowire, and then the position of single-layer defect was constructed in the gold nanowire according to the MPBP of the perfect nanowire. In this work (Fig. 1), the position of single-layer defect was constructed in the central plane of the nanowire (0.5 in the normalized nanowire). In the single-layer crystalline plane, vacancy defects were constructed to be in a uniform distribution according to vacancy ratio.

In MD calculations, the Verlet leapfrog algorithm was applied for the integration of motion equations to obtain velocity and trajectories of atoms. Nośe-Hoover thermostat was used as a rescaling method of velocity. Free boundary condition was adopted. For potential functions, tight-binding molecular dynamics (TB-MD) or Car-Parrinello molecular dynamics (CP-MD) simulations can give accurate results. However, these potential functions have some difficulty in calculating the nanowires with large size or many samples. Therefore, the embedded-atom method (EAM) potential developed by Johnson[31] might be the best choice for this particular purpose. Here, a statistical analysis and a series of comparisons were applied in the present study, which may also reduce the systematic error to ensure the reliability of MD simulations. The EAM potential developed by Johnson followed as:

$$E = \frac{1}{2}\sum_{ij} V(r_{ij}) + \sum_{i} F(\rho_i), \quad (1)$$

$$\rho_i = \sum_{i \neq j} \varphi(r_{ij}) \quad (2)$$

where E is the total internal energy of the system, V is the pair potential between atoms i and j, and r_{ij} is the distance between them, $F(\rho_i)$ is the energy to embed atom i in an electron density ρ_i, $\varphi(r_{ij})$ is the electron density at atom i due to

[a)] Corresponding author. Email: wangfenying@ncu.edu.cn.

atom j as a function of the distance r_{ij}. The stress (σ) in z-direction was calculated by the Virial scheme. All presented MD simulations and visualization processes were performed with a self-developed software NanoMD, and its reliability of algorithms has been validated not only by a large amount of theoretical simulations, but also with the comparison to the experimental measurements.

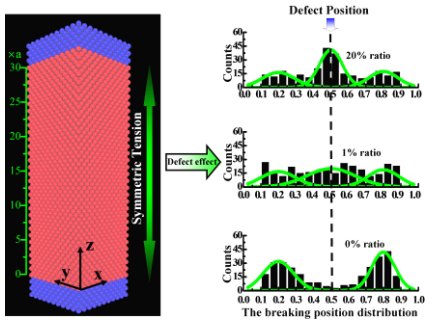

Fig. 1 Schematic illustration of theoretical models

RESULTS AND CONCLUSIONS

In this paper, MD simulations are used to study the influence of defects and temperature on the mechanical properties and the whole breaking process of the single-crystal gold nanowire subjected to symmetric stretching. It is found that: (i) increasing the applied temperature could lower the mechanical properties of the nanowires, and it results from the crystalline, local disorder, and amorphous deformations of the nanowires at low, middle and high temperatures, respectively. (ii) For the effects of defects on mechanical properties of the [100] oriented single-crystal gold nanowires, defects have improved the mechanical strength of the nanowire. Defects, to some extent, could prolong the elastic deformation of the nanowire at low temperature. (iii) The MPBP distributes at two ends of the nanowire at the temperatures from 5 to 750 K. When defects are constructed, the breaking of the nanowire behaves the sensitivity of defects when the defect ratio is 5% at 100 K. However, the defect ratio is 1% at 300 and 500 K. It is related with the deformation styles of crystalline structures at different temperatures.

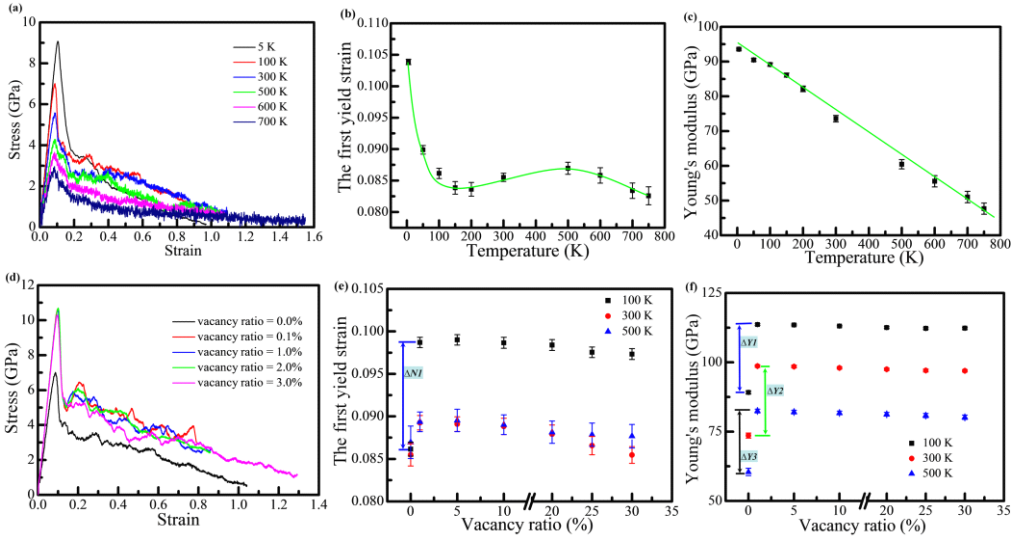

Fig. 2. The mechanical behaviors of the [100] oriented single-crystal gold nanowires at different temperatures. (a) The representative stress-strain relationship of the nanowire at the temperatures from 5 to700 K. (b) The first yield strain, (c) Young's modulus plotted against temperatures. (d) The stress-strain relationship with different vacancy ratios at 100 K. (e) The first yield strain, (f) Young's modulus plotted against vacancy ratios.

References

[1] Wang F., Gao Y., Zhu T., Zhao J., *Nanoscale* 2:2818, 2011.
[2] Wang F., Chen T., Zhu T., Gao Y., Zhao J., F. Y. Wang, *J. Appl. Phys.* 110:084307, 2011.
[3] Johnson R. A., *Phys. Rev. B* 39:12554-12559, 1989.